Supplement

Two Acridone Units in One Crown Ether

Incorporating a Second Acridone

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1 ^{1}H-NMR and ^{13}C-NMR spectra of the new compounds

Structural characterizations of the reported new compounds by NMR methods are shown in **Figs. S1–S17**.

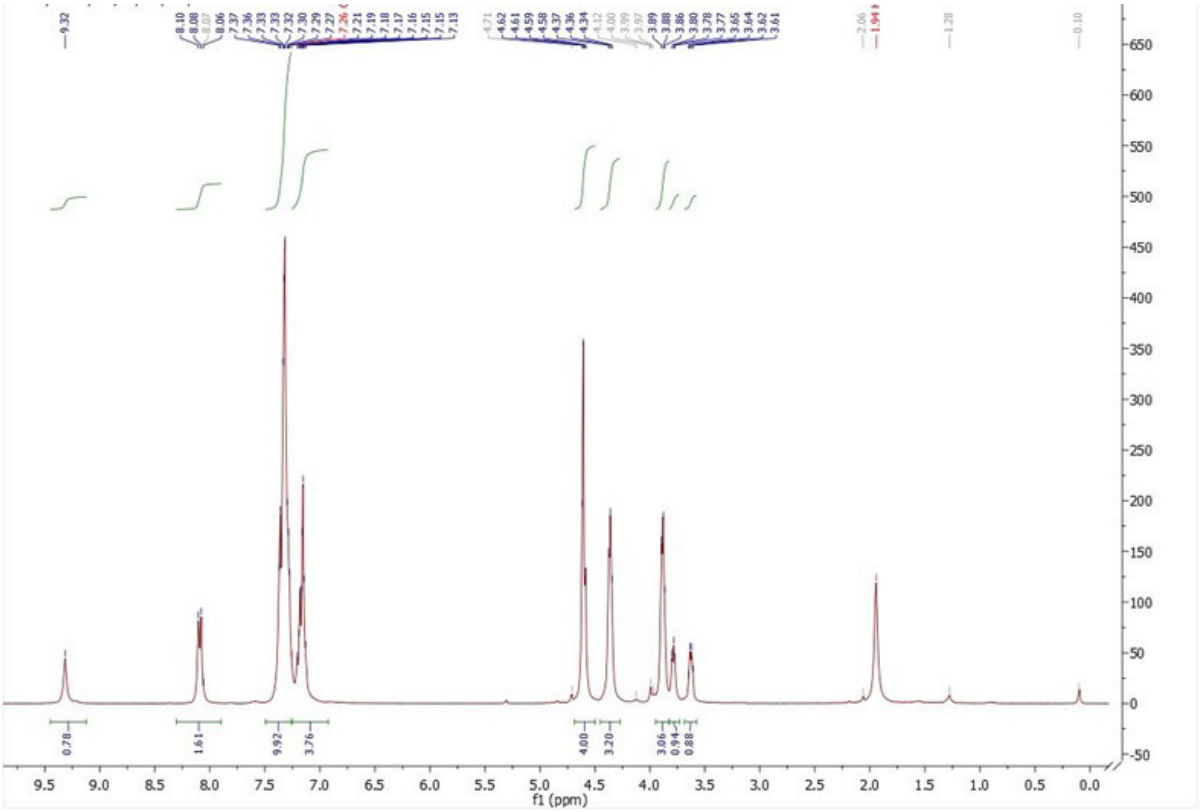

Fig. S1 ^{1}H-NMR spectrum of **6** (solvent: $CDCl_3$)

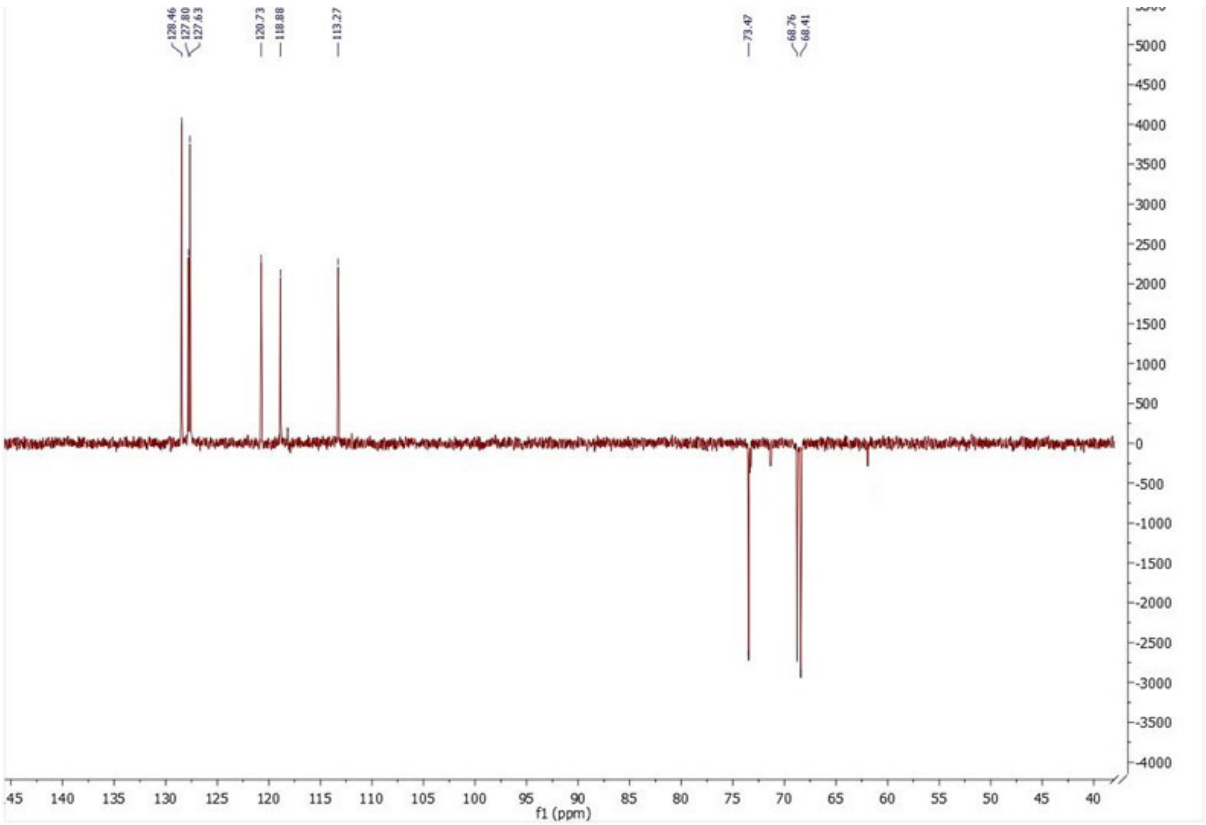

Fig. S2 ^{13}C-NMR spectrum of **6** (solvent: $CDCl_3$)

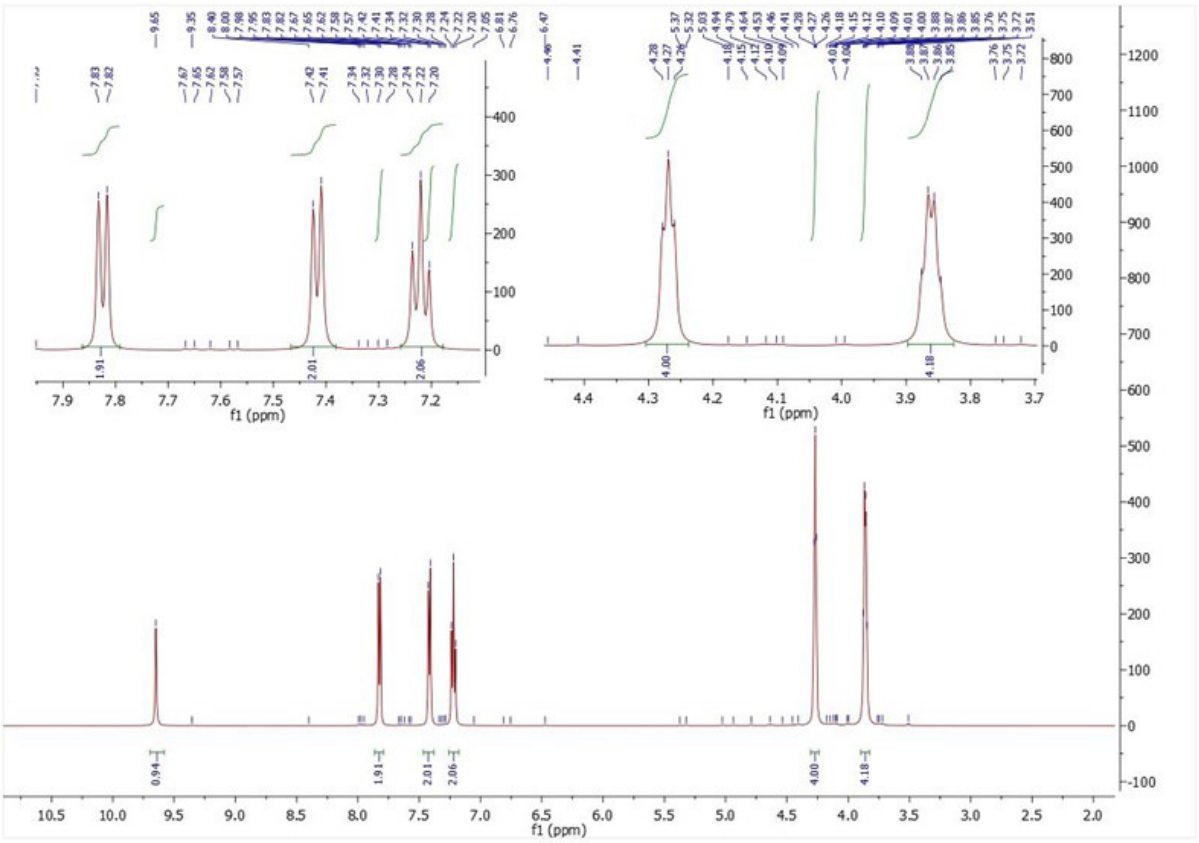

Fig. S3 ^{1}H-NMR spectrum of **8** (solvent: $(CD_3)_2SO$)

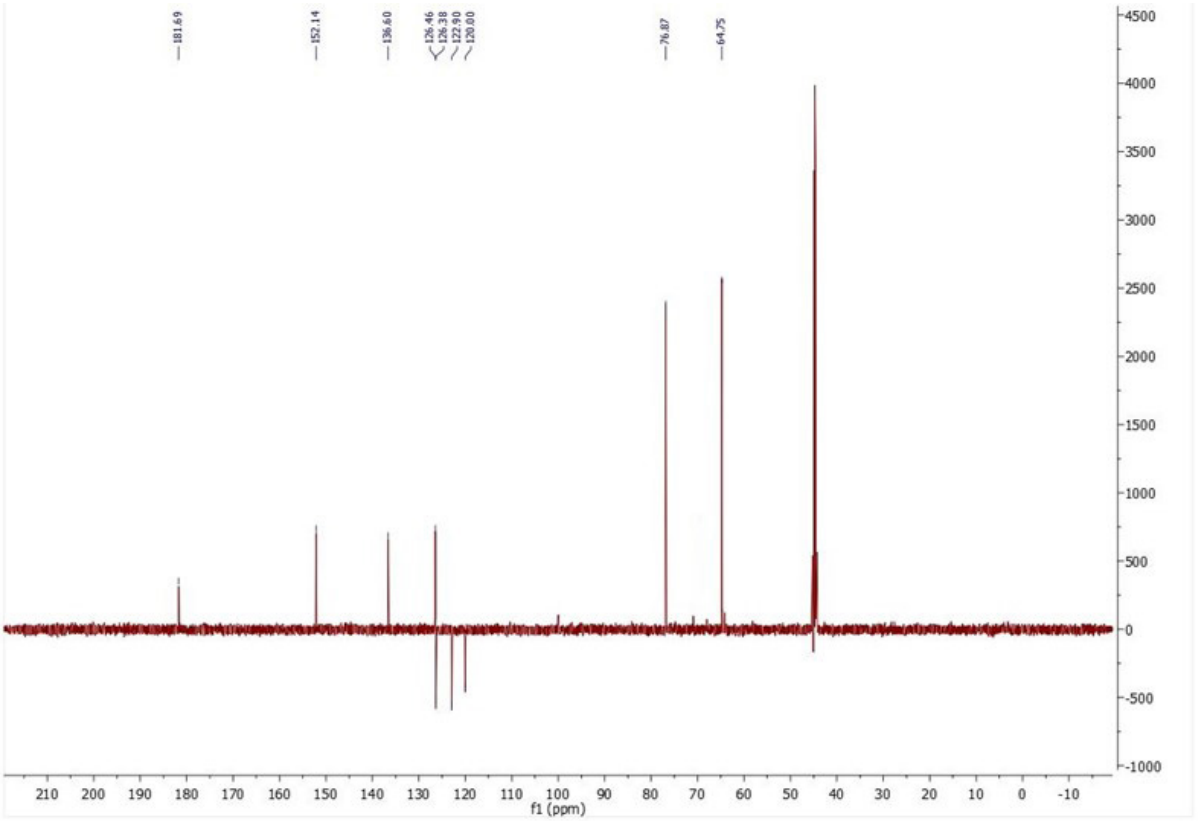

Fig. S4 ^{13}C-NMR spectrum of **8** (solvent: $(CD_3)_2SO$)

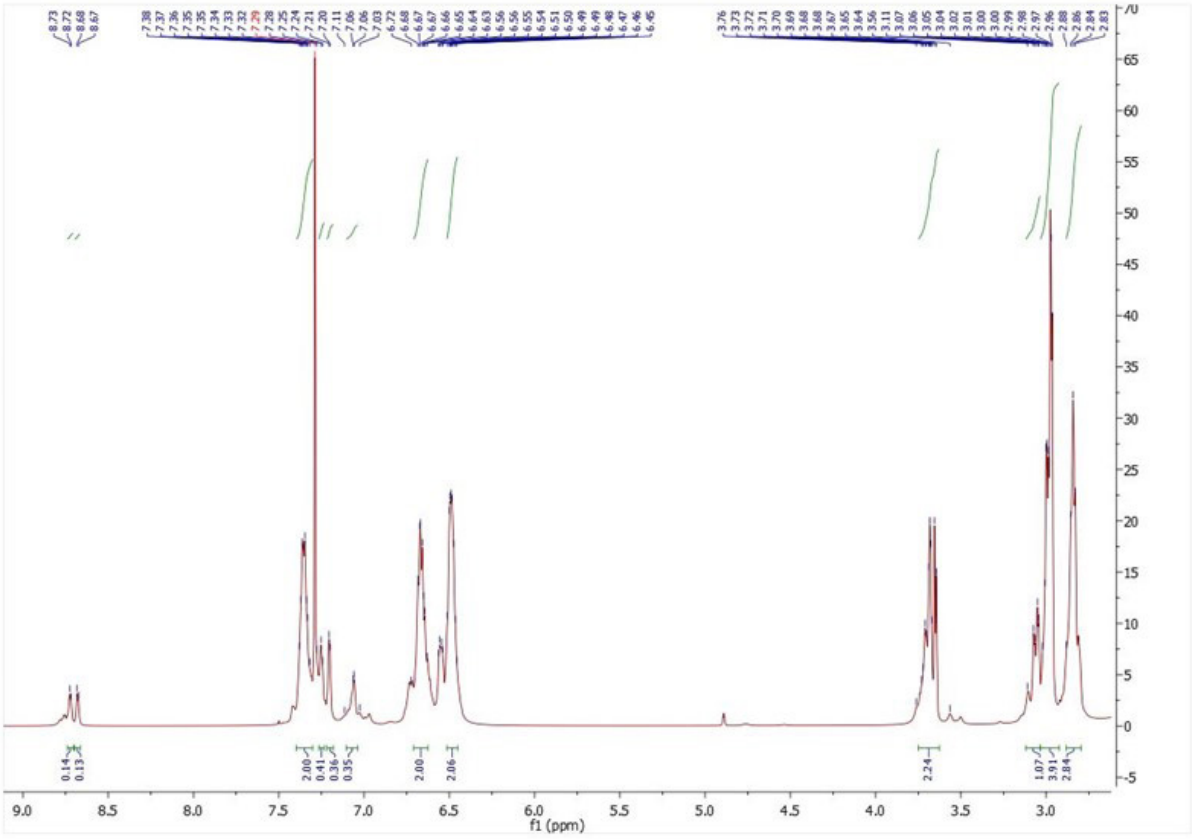

Fig. S5 ^{1}H-NMR spectrum of crude **10** (solvent: $CDCl_3$)

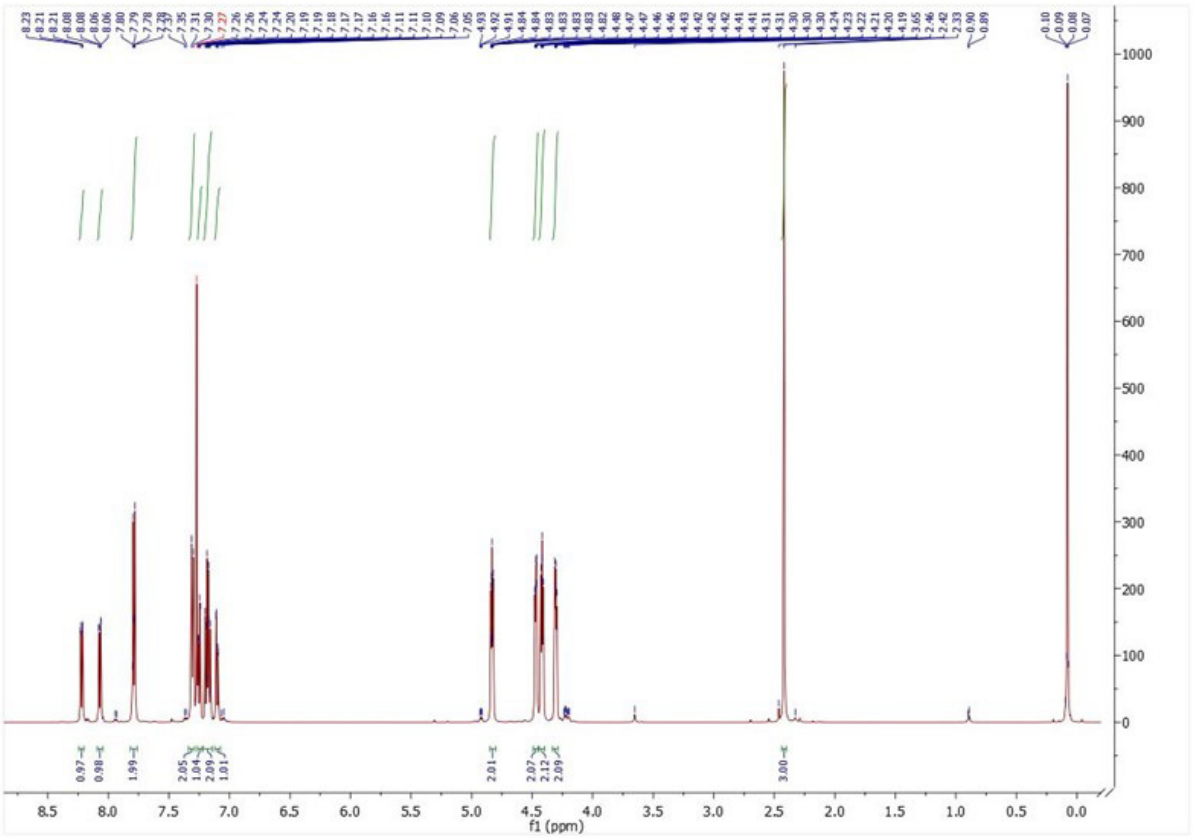

Fig. S6 ^{1}H-NMR spectrum of **12** (solvent: $CDCl_3$)

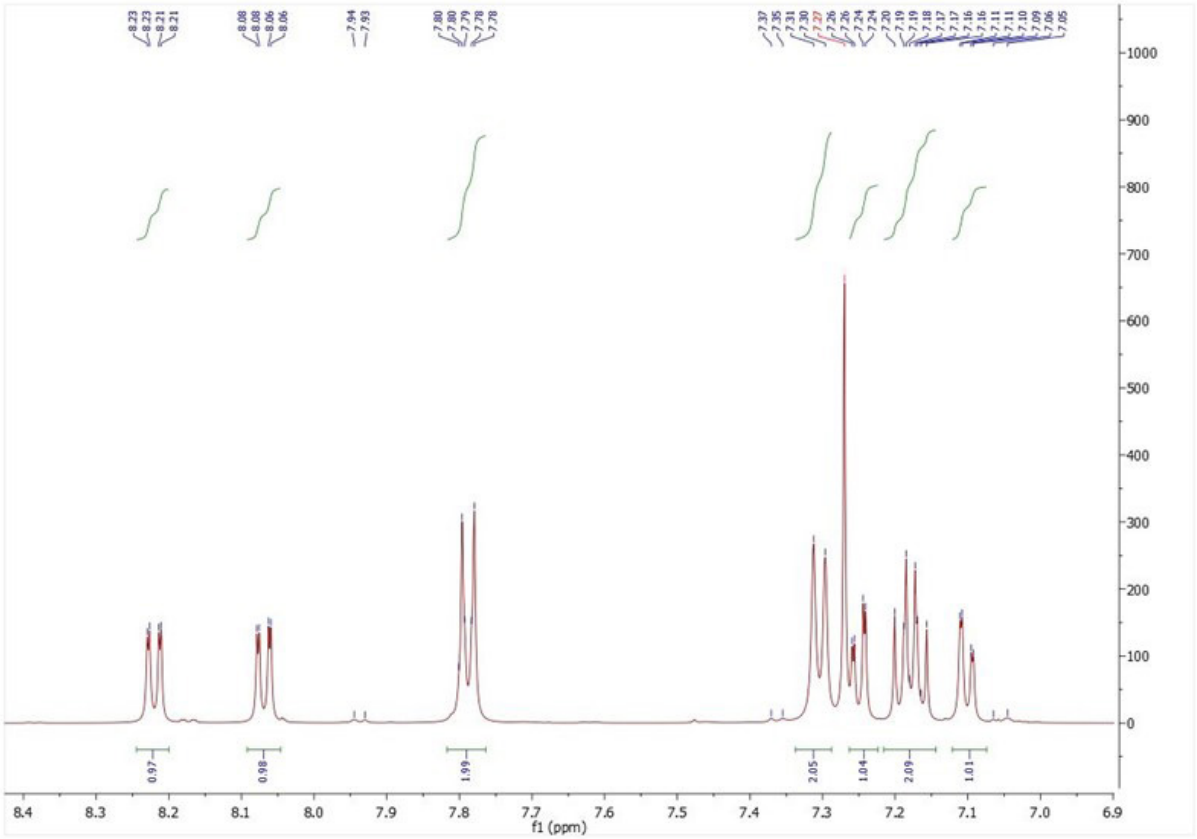

Fig. S7 ^{1}H-NMR spectrum of **12**, magnification of the aromatic signal range (solvent: $CDCl_3$)

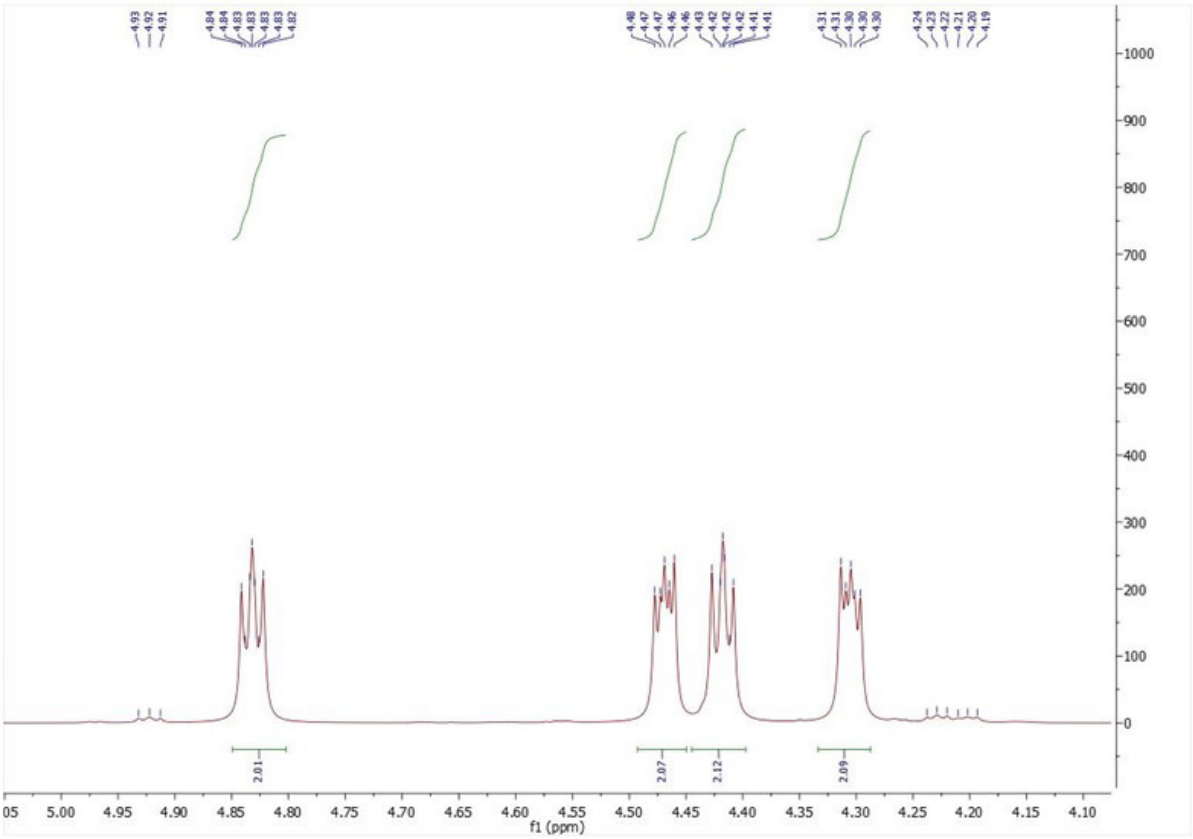

Fig. S8 ^{1}H-NMR spectrum of **12**, magnification of the ethereal signal range (solvent: $CDCl_3$)

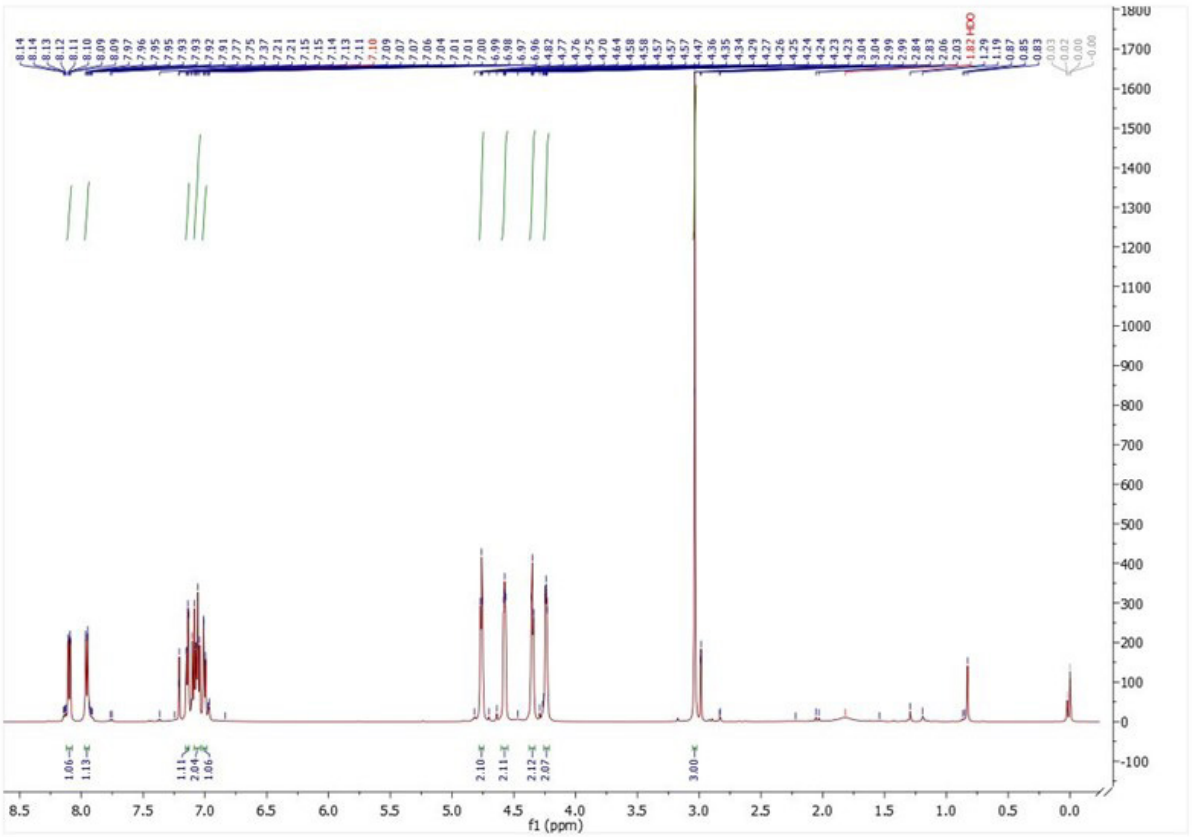

Fig. S9 ^{1}H-NMR spectrum of **13** (solvent: $CDCl_3$)

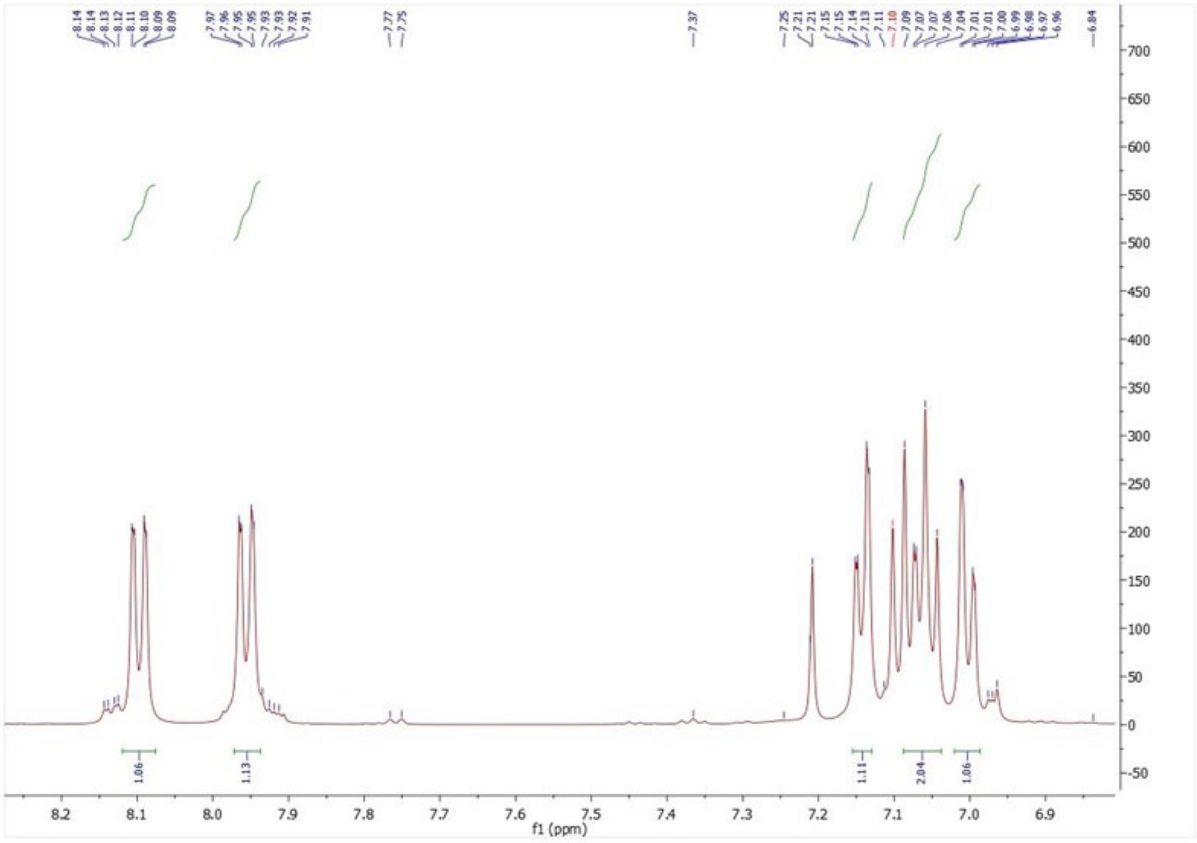

Fig. S10 ^{1}H-NMR spectrum of **13**, magnification of the aromatic signal range (solvent: $CDCl_3$)

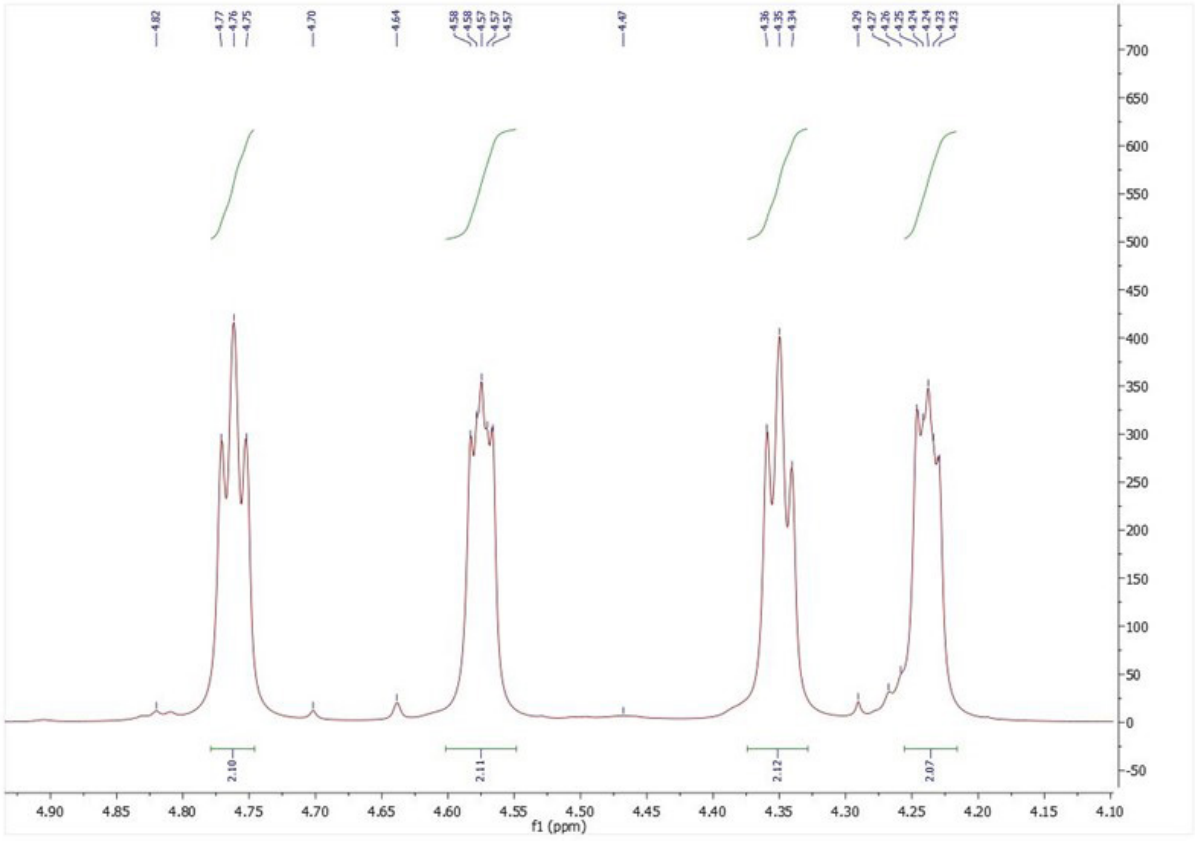

Fig. S11 ^{1}H-NMR spectrum of **13**, magnification of the ethereal signal range (solvent: $CDCl_3$)

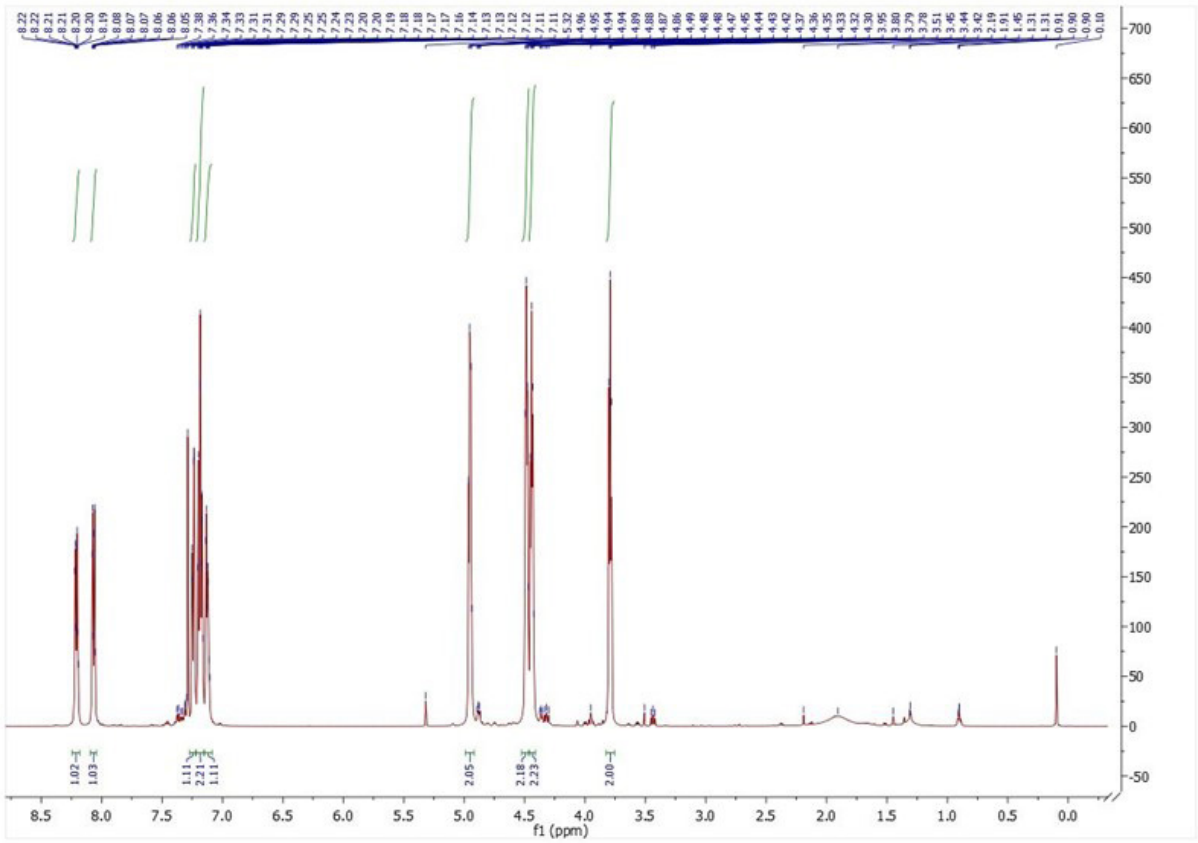

Fig. S12 ^{1}H-NMR spectrum of **14** (solvent: $CDCl_3$)

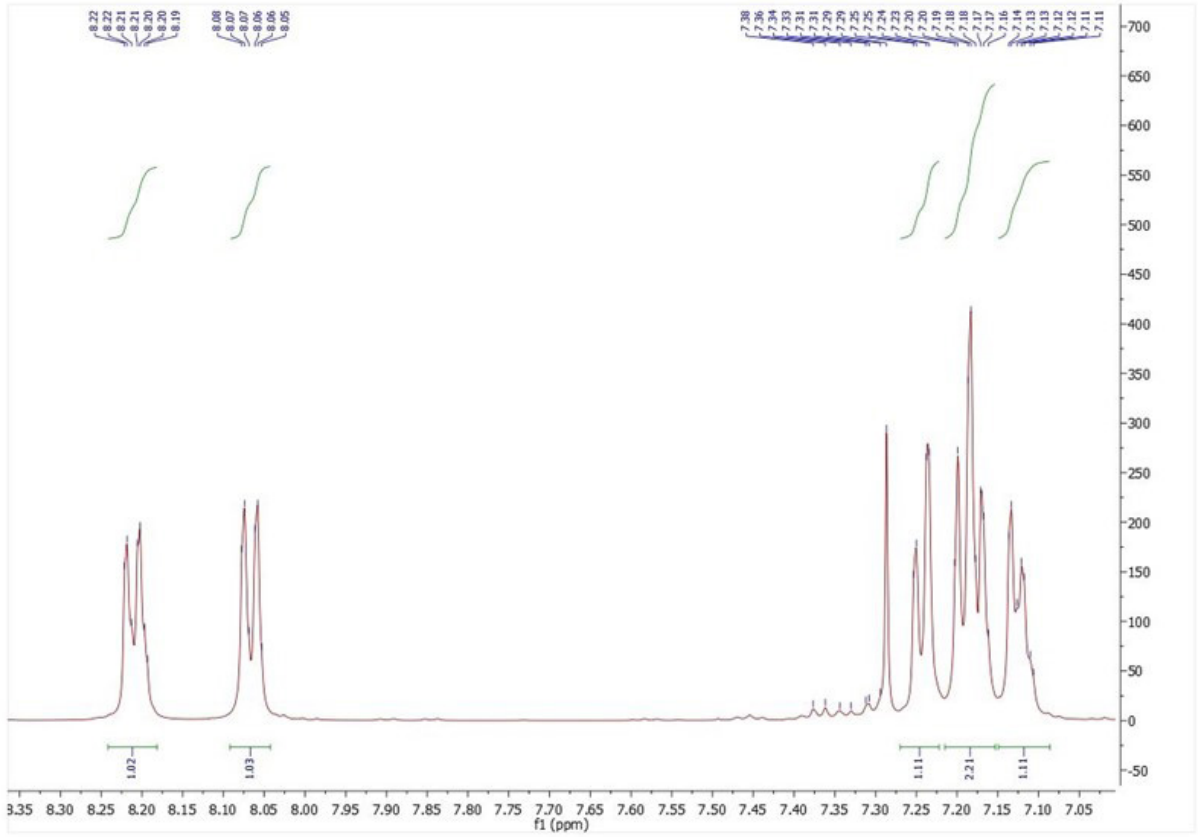

Fig. S13 ^{1}H-NMR spectrum of **14**, magnification of the aromatic signal range (solvent: $CDCl_3$)

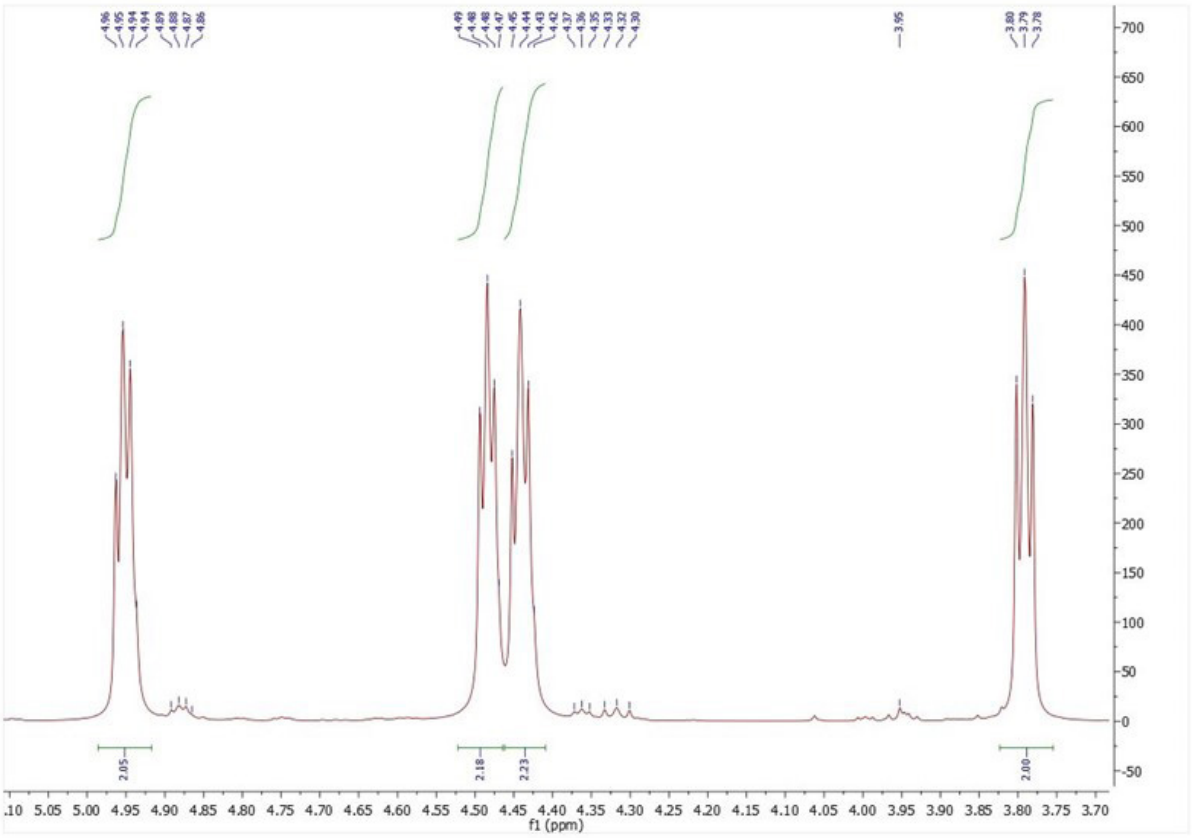

Fig. S14 [1]H-NMR spectrum of **14**, magnification of the ethereal signal range (solvent: $CDCl_3$)

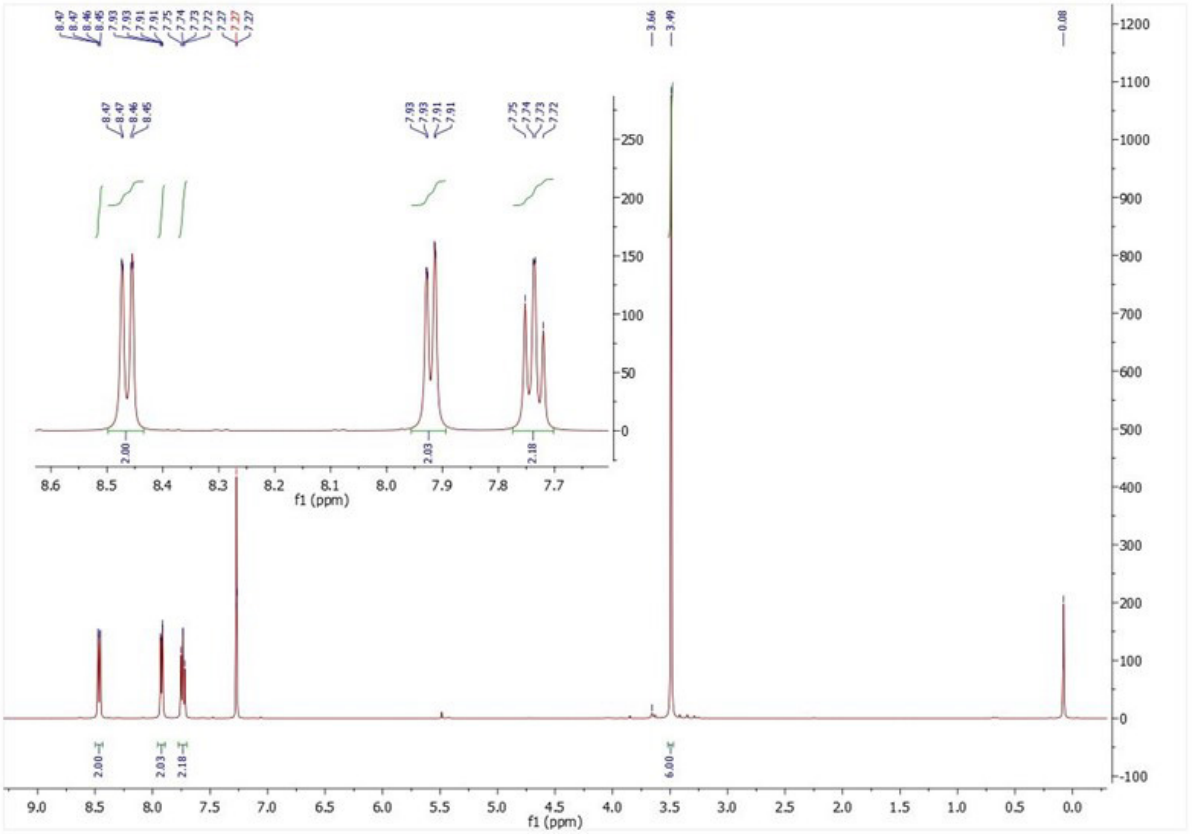

Fig. S15 [1]H-NMR spectrum of **21** (solvent: $CDCl_3$)

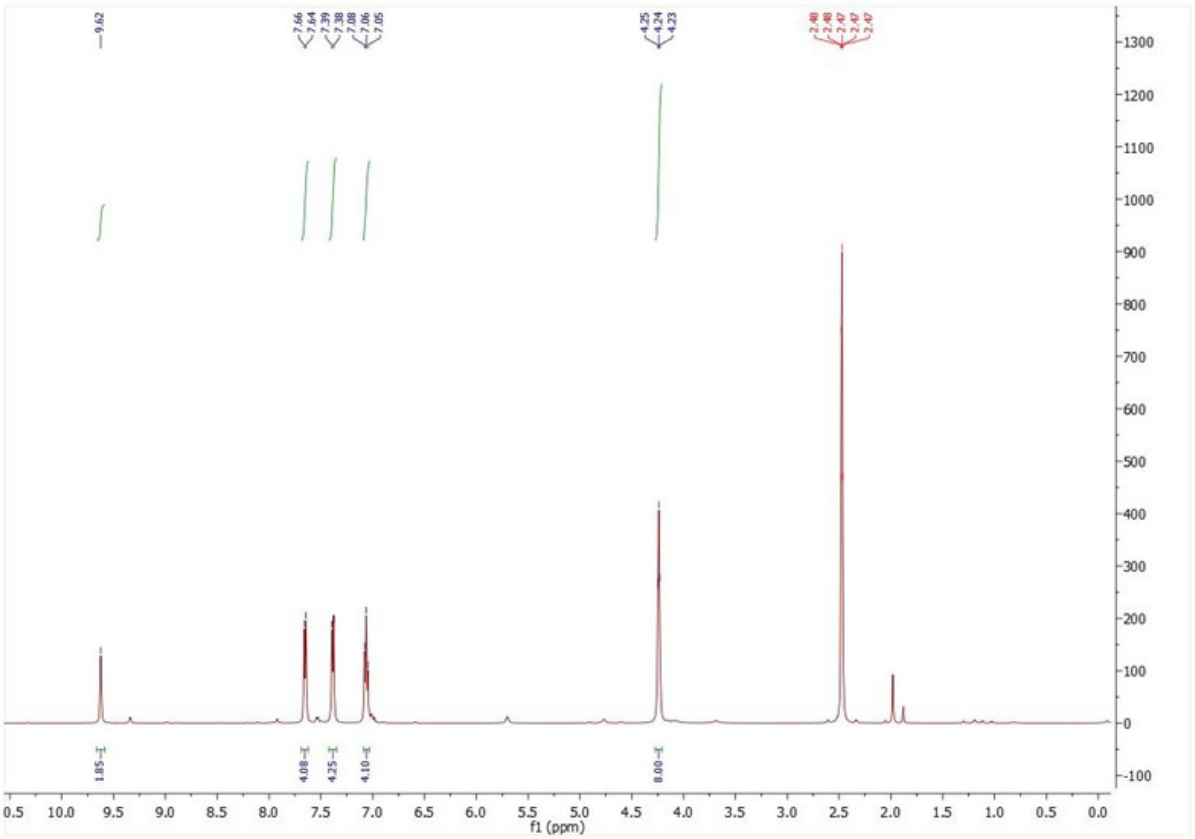

Fig. S16 ^{1}H-NMR spectrum of **11** (solvent: $(CD_3)_2SO$)

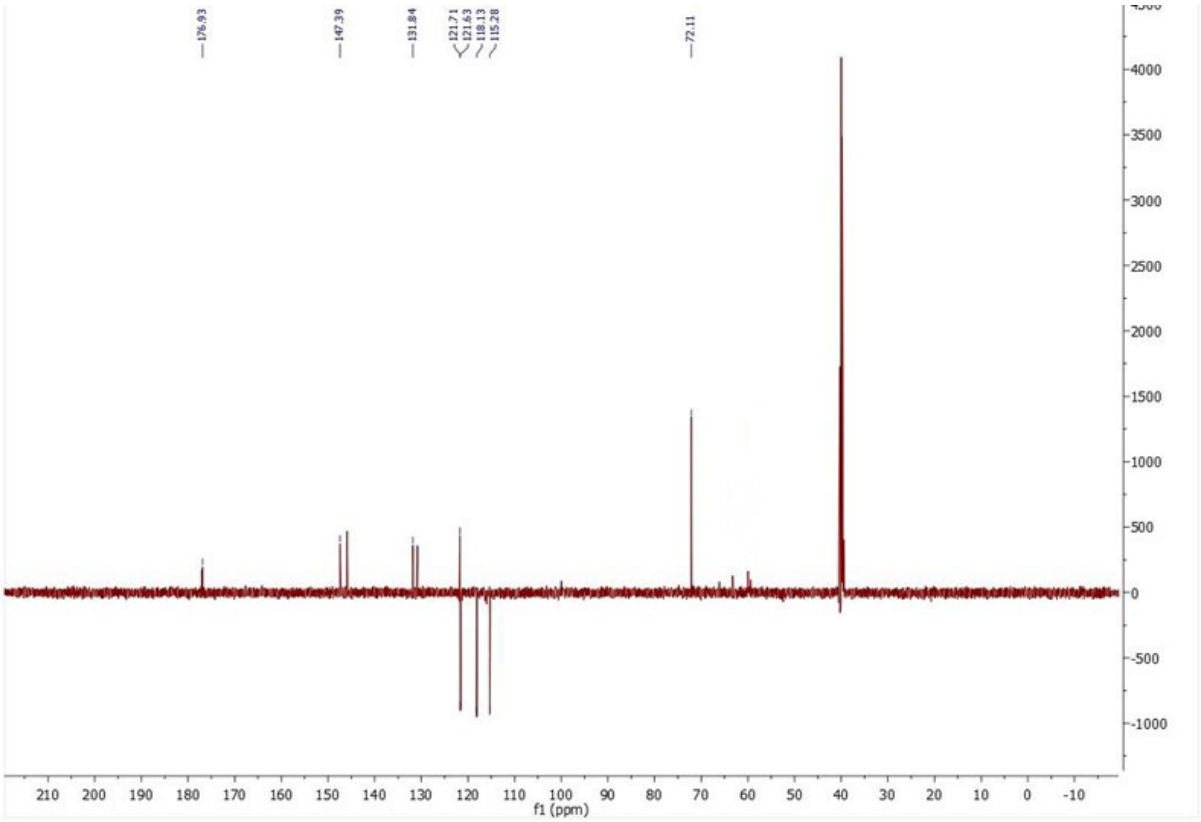

Fig. S17 ^{13}C-NMR spectrum of **11** (solvent: $(CD_3)_2SO$)

2 Theoretically estimated conformation and structural flexibility

Some basic calculations on conformation were made by using ChemAxon Conformer Plugin® software. The obtained lowest energy conformer of the molecule can be seen in **Fig. S18**.

We have also highlighted some of the other characteristic conformers of **11** with higher energy levels, which can be seen in **Fig. S19**.

It is reflected from the calculated energies of the conformers, that only a relatively little distortion of the structure is possible at room temperature. Even relatively small changes in the dihedral angles would result in large energetic differences (>100 kJ/mol, exceeding the typical energy barrier of atropisomers), thus the conversion between these conformers is strongly limited. According to the expectations, it indicates a rigid structure at room temperature. Rigid conformation and soft nucleophilic acridine-*N* atoms together result in high coordination and low differentiation ability toward soft electrophilic heavy-metal cations.

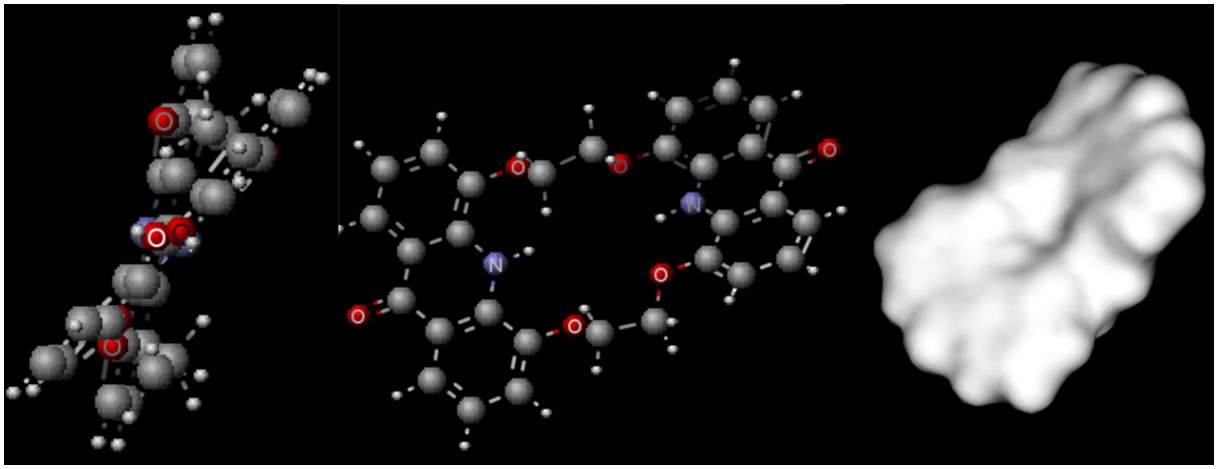

Fig. S18 The lowest energy conformer of the new bisacridono-crown ether **11** determined by ChemAxon Conformer Plugin® software (Fig. S18 shows different interpretations of the most stable conformer of a slightly twisted, almost planar 3D molecular structure; calculated energy: 425 kJ/mol)

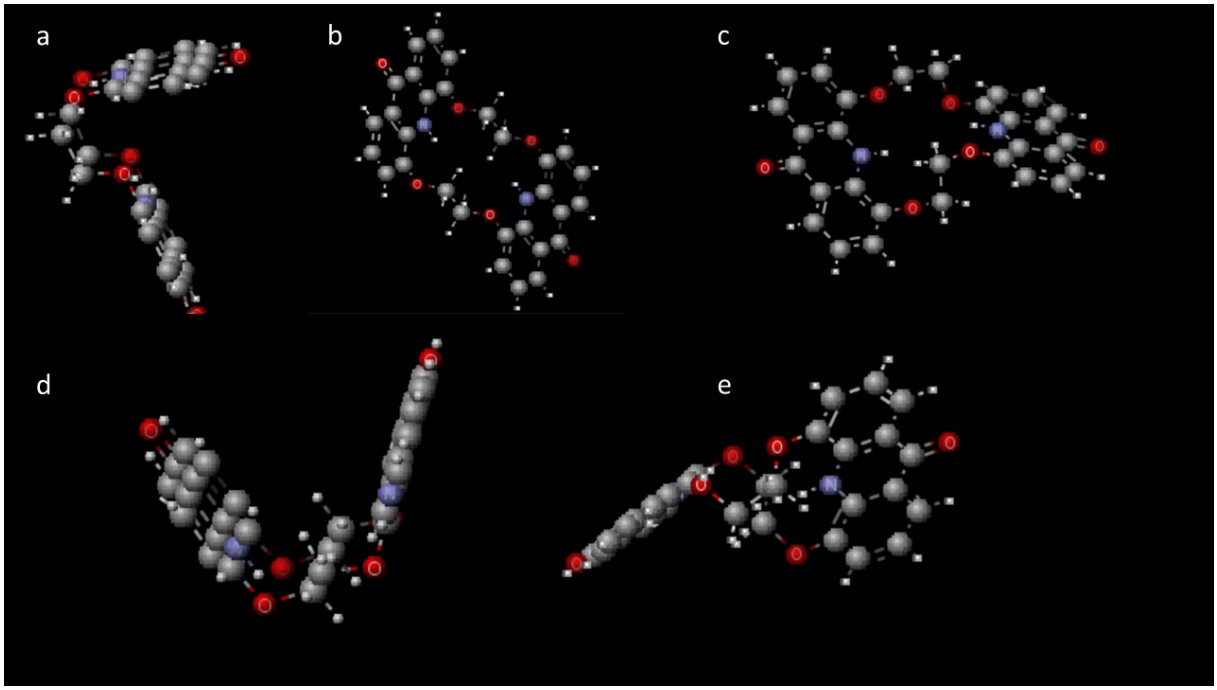

Fig. S19 Some less stable conformers (energy values calculated by ChemAxon Conformer Plugin® software for (a) chair-like conformer = 439 kJ/mol, for (b) fully planar conformer = 445 kJ/mol, for (c) partially twisted conformer = 449 kJ/mol, for (d) tub-like conformer = 530 kJ/mol, for (e) tightly twisted conformer = 532 kJ/mol

3 Spectrophotometric investigation of new macrocycle 11

The absorption and fluorescence emission spectra of the sensor molecule (**1**) are shown in **Figs. S20** and **S21**.

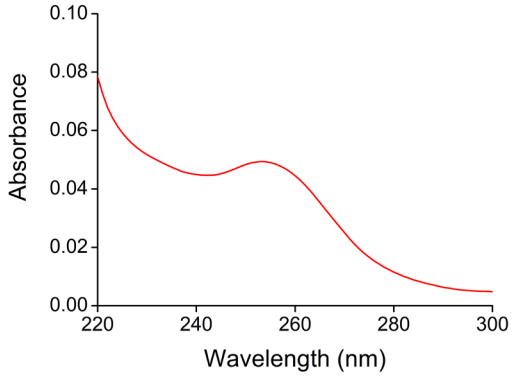

Fig. S20 UV/Vis absorption spectrum of new macrocycle **11** in acetonitrile

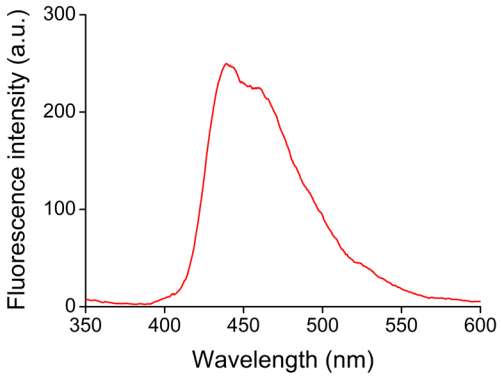

Fig. S21 Fluorescence emission spectrum of new macrocycle **11** in acetonitrile ($\lambda_{ex.}$ = 265 nm)